

# Symplectic parallel integrators in the realm of Hofer's geometry

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## Abstract

Symplectic integrators constructed from Hamiltonian and Lie formalisms are obtained as symplectic (indeed Hamiltonian) maps whose flow follows the exact solution of a “surrounded” Hamiltonian  $\tilde{H} = H + h^k H_1$ . Those modified Hamiltonians depends virtually on the time by the timestep size  $h$ . When the numerical integration of a Hamiltonian system involves more than one symplectic scheme as in the *parallel-in-time* algorithms and specifically the Parareal scheme, there are not a simple way to control the dynamical behavior of the error Hamiltonian. The interplay of two different symplectic integrators can degenerate their behavior if both have different dynamical properties, reflected in the number of iterations to have a good approximation to the final sequential solution. Considered as flows of time-dependent Hamiltonians we use the Hofer's geometry to search for the optimal coupling of symplectic schemes. As a result, we obtain the constraints in the Parareal method to have a good behavior for Hamiltonian dynamics.

## 1 Introduction

Symplectic integrators are the natural methods for simulating Hamiltonian dynamics. To construct a symplectic integrator, we can follow two different procedures: on one side we can use the Hamiltonian formalism using generating functions, Lie transforms, etc. On the other side we can take a general method, for instance, Runge-Kutta formulas, modifying the coefficients to satisfy the symplecticity conditions [1]. In general, we obtain implicit methods but when the Hamiltonian can be separated into kinetic and potential energies  $H(q, p) = T(p) - V(q)$  we can construct explicit methods easy to implement.

They are constructed using the diffeomorphisms which left invariant the symplectic form  $\omega = dp \wedge dq$  which defines the Hamiltonian vector field  $X_H$ . Such a diffeomorphisms are called symplectic diffeomorphisms or symplectomorphisms and they form a subgroup denoted by  $\text{Symp}(M, \omega)$ . In particular, the flow of any Hamiltonian vector field is a symplectic diffeomorphism and all of them form another subgroup of diffeomorphisms called the Hamiltonian diffeomorphisms, denoted by  $\text{Ham}(M, \omega)$ .

Moreover, using the Lie formalism we can consider  $\text{Symp}(M\omega)$  and  $\text{Ham}(M, \omega)$  as Lie groups and the sets of symplectic and Hamiltonian vector fields as their Lie algebras at the identity element. Then, for every Hamiltonian vector field  $X_H \in \mathfrak{ham}(M, \omega)$ , its flow is given by the exponential  $\varphi_t(x_0) = e^{tX_H}x_0$ . For a fixed  $t = h \in \mathbb{R}^+$  the mapping  $x(t_0) \mapsto x(t_0 + h)$  generated by  $\varphi_h = e^{hX_H}$  is a Hamiltonian map which defines the symplectic integrator. In fact, this is a Hamiltonian integrator which preserves more structure than the symplectic one.

Classically the parallelization of this type of systems is performed by a decomposition of the phase space (domain decomposition) or looking for parallelizable tasks into the method or into the equations. However, in the last two decades there were several attempts to develop another type of parallelization for symplectic integrators based on the decomposition of the time variable. The first attempt of some parallel-in-time algorithm for a scalar differential equation was published by Nievergelt in 1964 [39]. The idea is to decompose the total time in several subintervals which can be computed in parallel. Each interval, called a “branch”, must be modified propagating the corrected local initial condition to each subinterval; this technique has derived in the *multishooting* methods. Although the Nievergelt’s algorithm is not iterative, almost all other algorithms use an iterative process to approximate the sequential numerical solution. Those iterative algorithms consist in two steps: one *predictor* which estimates in parallel the value of several branches and one *corrector*<sup>1</sup> which approaches the final solution propagating the predictions between different branches. We call them the *time-parallel* algorithms and all of them differ in the corrector step which uses different iterative process to convergence. Of course, there are others differences but in this paper we are interested in the corrector step.

As noted by Saha, Stadel and Tremaine [44] one way to time-parallelize an almost integrable Hamiltonian system is to compute in parallel several branches saving the perturbing contributions and to propagate them computing in sequence the integrable Hamiltonian part. This technique is reproduced in [26] for high-order symplectic integrators however, it works fine if the ratio of the computing time of the integrable over the perturbing part is very small. This approach is very accurate but expensive. On the other extreme, there is the *parareal* method introduced by Lions, Maday and Turinici in [33] and refined in [4]. In this method the propagation of the predictions is made by a simple increment of the corrector at every iteration. As a result, it is a very fast algorithm, however, for Hamiltonian systems there are several inconvenients associated to the non preservation of the geometric structure of the underlying integrators.

In order to deal with this type of problems, Bal and Wu [5] have done the first step considering a new way to spread the information between branches in the sequential step and practically destroying the “pure” parareal scheme. Also, Dai *et al.* [12] have introduced another variation of the parareal step, using symmetries and projections into the energy manifold to preserve the geometric

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<sup>1</sup>Many authors inverse the terminology considering the parallel step as the corrector and the sequential step as the predictor. Our choice is evident when we relate the corrector step with the *symplectic correctors* studied in [50, 37, 38]

properties of the underlying integrators. Recently, the author has proposed a geometric corrector step using Lie's algebras [28] which is equivalent to that from Dai *et. al.*. In this paper we translate that approach to the Hofer's geometry in order to search not only for Hamiltonian maps but for optimizing the energy (which we relate with the number of iterations) to go from the first guess solution to the final solution.

## 2 Lie algebras and Hamiltonian vector fields

We consider the phase space of a Hamiltonian system as a symplectic manifold<sup>2</sup>  $M = T^*\mathbb{R}^n \cong \mathbb{R}^{2n}$  with the canonical symplectic form  $\omega = dp \wedge dq$ . Denote by  $\mathfrak{X}(M)$  the set of all vector fields and by  $\mathfrak{F}(M) \cong C^\infty(M)$  the set of all smooth functions over  $M$ .

We define de binary operation  $[\cdot, \cdot] : \mathfrak{X}(M) \times \mathfrak{X}(M) \rightarrow \mathfrak{X}(M)$  by the rule

$$[X, Y] = XY - YX, \quad X, Y \in \mathfrak{X}(M), \quad (1)$$

called the Lie bracket, which is: bilinear, alternating, and satisfies the Jacobi identity. The set of all the vector fields  $\mathfrak{X}(M)$  equipped with the Lie bracket (1) obtains the structure of Lie algebra  $(\mathfrak{X}(M), [\cdot, \cdot])$ .

Let  $\mathcal{L}_X F$  be the Lie derivative of  $F$  along the vector field  $X \in \mathfrak{X}(M)$ .  $\mathcal{L}_X F$  measures the change of  $F$  along  $X$  where  $F$  can be a function, a vector field, a  $p$ -form or, in general, a tensor.

The Lie derivative of the symplectic form  $\omega$  along  $X$  is given by the Cartan's magic formula

$$\mathcal{L}_X \omega = di_X \omega + i_X d\omega, \quad (2)$$

where  $d$  is the exterior differential and  $i_X \omega = \omega(X, \cdot)$  is the contraction of  $\omega$  by  $X$  or equivalently the inner product of the vector field  $X$  with the 2-form  $\omega$ .

We say that the vector field  $X$  is *symplectic* if its flow preserves  $\omega$ , which means  $\mathcal{L}_X \omega = 0$ . Since  $\omega$  is the canonical symplectic 2-form then  $\omega = -d\lambda$  where  $\lambda = pdq$  is the Liouville form. Consequently, the second term in the right hand side of (2) is zero. In other words, a vector field  $X$  is symplectic if the 1-form  $i_X \omega$  is closed which means that it belongs to the kernel of  $d$

$$d(i_X \omega) = d(\omega(X, \cdot)) = 0.$$

We denote the set of symplectic vector fields on  $M$  by  $\mathfrak{sp}(M, \omega)$ .

We say that  $X$  is *Hamiltonian* if, in addition,  $i_X \omega$  is exact, *i. e.*, there exists  $f \in \mathfrak{F}(\mathbb{R}^{2n})$  such that

$$i_X \omega = \omega(X, \cdot) = -df. \quad (3)$$

We call  $f$  a Hamiltonian function for  $X$  and we write  $X = X_f$  to specify that  $X$  is the Hamiltonian vector field associated to  $f$ . the set of all Hamiltonian vector

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<sup>2</sup>All the computations and results listed here apply to arbitrary symplectic manifolds  $(M, \omega)$ .

fields on  $M$  is denoted by  $\mathfrak{ham}(M, \omega)$ . Finally, the triplet  $(M, \omega, X_H)$  defines a Hamiltonian system over  $M$ . For general mechanical systems the configuration space can be consider as a Riemannian manifold  $(N, g)$  and the phase space becomes the cotangent bundle  $M = T^*N$  which has a natural structure of symplectic manifold.

We need a non obvious result from the theory of differential  $p$ -forms which give us the expression of the inner product of the Lie bracket with a  $p$ -form  $\alpha$  over any differential manifold  $M$ . The inner product  $i_{[X,Y]}\alpha$  for any  $p$ -form  $\alpha$  is given by ([7, pp 73]):

$$i_{[X,Y]}\alpha = \mathcal{L}_X(i_Y\alpha) - i_Y(\mathcal{L}_X\alpha).$$

Consequently, for every two  $X, Y \in \mathfrak{sp}(M, \omega)$  we have

$$\begin{aligned} i_{[X,Y]}\omega &= \mathcal{L}_X(i_Y\omega) + 0 \\ &= d(i_X(i_Y\omega)) + 0 \\ &= d(\omega(Y, X)) \\ &= -d(\omega(X, Y)) \end{aligned}$$

where we used  $\mathcal{L}_Y\omega = 0$  and  $d\omega = 0$ .

These computations has important consequences: 1)  $[X, Y]$  is a Hamiltonian vector field. 2) Since  $\mathfrak{ham}(M, \omega) \subset \mathfrak{sp}(M, \omega)$ , the Lie bracket  $[\cdot, \cdot]$  gives them the structure of Lie subalgebras of  $\mathfrak{X}(M)$ , and 3)  $\mathfrak{ham}(M, \omega)$  is an (in fact the maximal) ideal of  $\mathfrak{sp}(M, \omega)$  with respect to  $[\cdot, \cdot]$ , *i.e.*

$$[\mathfrak{sp}(M, \omega), \mathfrak{sp}(M, \omega)] \subset \mathfrak{ham}(M, \omega).$$

We have the relations

$$\mathfrak{ham}(M, \omega) \subset \mathfrak{sp}(M, \omega) \subset \mathfrak{X}(M). \quad (4)$$

It is a well-known fact that  $\mathfrak{ham}(M, \omega) = \mathfrak{sp}(M, \omega)$  if and only if the fundamental group of  $M$  is trivial; in other words, when  $M$  is simply connected.

Now we link this point of view with the classical development in local coordinates. Let  $H : M \rightarrow \mathbb{R}$  be a differentiable function with Hamiltonian vector field  $X_H$  on  $M$ . Select a point  $v \in \phi^{-1}(M)$  in a local chart of  $M$ . The Darboux's theorem says that, locally, all symplectic manifolds are symplectomorphic to  $T^*\mathbb{R}^n \cong \mathbb{R}^{2n}$  and then we can consider that  $v \in \mathbb{R}^{2n}$ . In canonical symplectic coordinates  $v = (q, p)$  such that  $q \in \mathbb{R}^n$  and  $p \in T_q^*\mathbb{R}^n \cong \mathbb{R}^n$ . The vector field  $X_H$  in local coordinates is

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}, \quad (5)$$

which are called the Hamilton equations.

For two differentiable functions  $f, g \in \mathfrak{F}(M)$ , their associated Hamiltonian vector fields  $X_f, X_g$  fullfils  $\omega(X_f, X_g) = -\{f, g\}$  where  $\{\cdot, \cdot\}$  is the *Poisson bracket* for functions defined by

$$\{f, g\} := \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial g}{\partial q} \frac{\partial f}{\partial p}. \quad (6)$$

The binary operation (6) is bilinear, antisymmetric and fulfills the Jacobi identity. The space of real-valued differentiable functions  $\mathfrak{F}(M)$ , equipped with the Poisson bracket (6), obtains the structure of Lie algebra. It is possible to write the Hamiltonian vector field in terms of the Poisson brackets by

$$\dot{z} = X_H(z) = \{z, H\}.$$

There exists a natural anti-morphism of Lie algebras between the algebra of differentiable functions  $\mathfrak{F}(M, \{\cdot, \cdot\})$  and the algebra of Hamiltonian vector fields  $\mathfrak{X}(M, [\cdot, \cdot])$  given by

$$f \mapsto X_f \tag{7}$$

$$\{f, g\} \mapsto X_{\{f, g\}} = -[X_f, X_g] \tag{8}$$

Since the Poisson bracket of two functions is a function then the Lie bracket of two Hamiltonian vector fields is again a Hamiltonian vector field, as we have shown before.

### 3 Hamiltonian diffeomorphisms and Hofer's geometry

A symplectic diffeomorphism or symplectomorphism of a symplectic manifold  $(M, \omega)$  is a  $C^\infty$  diffeomorphism  $\phi \in \text{Diff}(M)$  which preserves the symplectic structure  $\omega$ , it means that the *pull-back* of  $\phi$  fulfills  $\phi^*(\omega) = \omega$ . The support of a diffeomorphism  $\phi$  is the closure of  $\{x \in M | \phi(x) \neq x\}$ . The set of all symplectomorphisms with compact support form a group, denoted  $\text{Symp}(M, \omega)$  (with the law of composition of mappings).

Let  $X_H \in \mathfrak{ham}(M, \omega)$  be a Hamiltonian vector field. The flow  $\varphi_t^H = e^{tX_H}(x_0)$  of  $X_H$  is a one parameter subgroup of symplectic diffeomorphisms<sup>3</sup>. The set of all the symplectomorphisms which arise as the flow  $\varphi_t^f$  of Hamiltonian vector fields  $X_f$  form another subgroup of diffeomorphisms called the Hamiltonian diffeomorphisms, denoted by  $\text{Ham}(M, \omega)$ . It is easy to prove that  $\text{Ham}(M, \omega)$  is an infinite-dimensional subgroup since for every  $f \in \mathfrak{F}(M)$ , we have a mapping  $X_- : \mathfrak{F}(M) \rightarrow \mathfrak{X}(M)$  which maps  $f \mapsto X_f$  with  $\ker(X_-) \cong \mathbb{R}$  the constant functions. The exponential map  $e^- : \mathfrak{ham}(M, \omega) \rightarrow \text{Ham}(M, \omega)$  is injective then the composition  $e^- \circ X_-(H) = e^{tX_H}$  sends an infinite dimensional basis of  $\mathfrak{F}(M)$  to an infinite-dimensional basis of  $\text{Ham}(M, \omega)$ .

We can relate the groups  $\text{Ham}$ ,  $\text{Symp}$  and  $\text{Diff}$  with the Lie algebras in (4) by the exponential map as follows

$$\begin{array}{ccccccc} \text{Ham}(M, \omega) & \subset & \text{Symp}(M, \omega) & \subset & \text{Diff}(M) \\ \exp \uparrow & & \exp \uparrow & & \exp \uparrow \\ \mathfrak{ham}(M, \omega) & \subset & \mathfrak{sp}(M, \omega) & \subset & \mathfrak{X}(M). \end{array} \tag{9}$$

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<sup>3</sup>We use the exponential map of vector fields since  $\text{Symp}(M, \omega)$  is actually a Lie group

The reader must note that the exponential mapping is, in general, not surjective and the group  $\text{Symp}(M, \omega)$  can have several components. By construction  $\text{Ham}(M, \omega)$  belongs to the identity component of  $\text{Symp}(M, \omega)$ .

Consider the set of time-dependent Hamiltonian functions  $H : M \times I \rightarrow \mathbb{R}$  with compact support. We can *normalize* such a function since for every interval  $I = [0, a], a < \infty$  the flow of the vector field associated to the function  $\tilde{H}(x, t) = aH(x, at)$  defined on  $\tilde{I} = [0, 1]$  is again a Hamiltonian flow. More generally for every smooth function  $g(t)$  with  $g(0) = 0$  the flow  $\varphi_{g(t)}^H$  is Hamiltonian with normalized Hamiltonian function  $\frac{dg}{dt}(t)H(x, g(t))$  [41]. These properties of rescaling in time are used to regularize singularities in mechanical systems.

We can restate the definition of Hamiltonian diffeomorphism in the following way: a *Hamiltonian diffeomorphism* is a diffeomorphism  $\phi : M \rightarrow M$  which can be written as the time-1-map of a Hamiltonian flow, *i.e.*,  $\phi = \varphi_1^H$  for some time-periodic Hamiltonian  $H : \mathbb{S}^1 \times M \rightarrow \mathbb{R}$  [45]. Let us denote by  $H_t$  the function  $H(t, \cdot)$  on  $M$ . In the following, we will normalize the Hamiltonians and consider only the time-1-maps in  $\text{Ham}(M, \omega)$ . We denote by  $\mathcal{H}(M, \omega)$  the group of time-1-map of Hamiltonian flows which is a subgroup of  $\text{Ham}(M, \omega)$ .

**Remark 1.** *There is a constraint in all these definitions since the theory applies for functions and diffeomorphisms with compact support. However, for symplectic integrators, we do not need global properties and the most important thing is the numerical tests for the error behavior.*

A diffeomorphism  $\phi \in \text{Diff}(M)$  is said to be *isotopic to the identity* if there exists a smooth map  $H : M \times [0, 1] \rightarrow M$  such that if  $h_t : M \rightarrow M$  is given by  $h_t(x) = H(x, t)$ , then  $h_t$  is a  $C^\infty$  diffeomorphism,  $h_0 = \text{id}_M$  and  $h_1 = \phi$ . We say that  $h_t$  is an isotopy from  $\phi$  to the identity.

We say that  $h_t$  is a *Hamiltonian isotopy* if there exists a smooth family of functions  $H_t : M \rightarrow \mathbb{R}$  such that

$$i_{X_{h_t}}\omega = -dH_t \quad (10)$$

In this way, we have constructed curves or trajectories in  $\text{Ham}(M, \omega)$  which connects any Hamiltonian diffeomorphism in  $\mathcal{H}(M, \omega)$  with the identity map.

For every  $\phi \in \text{Ham}(M, \omega)$ , choose a Hamiltonian isotopy  $\Phi = (\phi_t)$  from  $\phi$  to the identity. Hofer [24] defined the length of this isotopy by

$$l_H(\Phi) := \int_{\mathbb{S}^1} \text{osc}(H_t) dt \quad (11)$$

where  $\text{osc}(H_t) := \max(H_t) - \min(H_t)$  denotes the oscillation of a function on  $M$ . For  $H \in \mathcal{H}(M, \omega)$ , it is clear that  $l(H) = 0$  if, and only if,  $H = 0$ . The *distance from the identity*, or *energy*, of an element  $\phi \in \text{Ham}(M, \omega)$  is defined as

$$d(\text{id}, \phi) := \inf\{l(H) | H \in \mathcal{H}, \phi = \varphi_1^H\}. \quad (12)$$

Let us extend the distance to a function  $d : \text{Ham}(M, \omega) \times \text{Ham}(M, \omega) \rightarrow [0, \infty)$  by setting  $d(\phi, \psi) := d(id, \psi \circ \phi^{-1})$ . Hofer has showed in [23] that  $d(\cdot, \cdot)$  is a bi-invariant metric on  $\text{Ham}(M, \omega)$  defined intrinsically. Then the set  $\text{Ham}(M, \omega)$  with the metric (12) is called the Hofer's geometry and it is a fundamental stone in symplectic topology.

As was pointed out by Siburg in [45], to every Hamiltonian dynamical system corresponds one single path in  $\text{Ham}(M, \omega)$  and vice versa. All the dynamical properties of the Hamiltonian system, including its periodic orbits, heteroclinic connections, etc. are contained in the Hamiltonian isotopy. Moreover, Baily and Polterovich have showed in [8] that the bifurcation diagram of every Hamiltonian system is preserved for every Hamiltonian diffeomorphism contained in a geodesic path in  $\text{Ham}(M, \omega)$ .

For instance, let  $H_t \in \mathcal{H}(M, \omega)$  be an admissible Hamiltonian which means that  $H_t$  has a compact support for every  $t \in I$ . Then  $H_t$  is said to *generate a minimal geodesic* if  $d(id, \varphi_t^H) = l(H)$ . However, it is very difficult to work with the space of geodesics in  $\text{Ham}(M, \omega)$ .

## 4 Symplectic integrators and Hamiltonian maps

Symplectic integrators are the natural numerical methods for simulating Hamiltonian dynamics. From the geometrical point of view, the most natural integrators are obtained by the Hamiltonian formalism and the Lie theory applied to the group  $\text{Ham}(M, \omega)$  and its Lie algebra  $\mathfrak{ham}(M, \omega) \cong T_{Id}(\text{Ham}(M, \omega))$ .

Consider the Hamiltonian system  $(M, \omega, X_H)$ . The flow generated by the Hamiltonian vector field  $X_H \in \mathfrak{ham}(M, \omega)$  is the one-parameter subgroup of  $\text{Ham}(M, \omega)$  defined by  $\varphi_t^H(x_0) = e^{tX_H}(x_0)$  where  $x_0 \in M$  is the initial condition of the vector field. For a fixed value  $t = \tau$  the mapping  $e^{\tau X_H} : M \rightarrow M$  is a symplectic, actually a Hamiltonian map. In the generic case,  $e^{\tau X_H}$  is very complicated and is given in (analytical) implicit form.

However, there exists an important class of Hamiltonian functions for which the Legendre condition<sup>4</sup> is satisfied. This class is formed by separable functions  $H(q, p) = T(p) + V(q)$  where  $T(p)$  is the kinetic energy and  $V(q)$  is the potential. (We use the plus sign in order to develop the exponential as a product.) Then the Hamiltonian vector field is separable and each part can be integrated independently obtaining an implicit method. If we write  $X_H = X_T + X_V$  the flow generated by  $X_H$  becomes

$$\varphi_t^H = e^{\tau X_H} = e^{\tau(X_T + X_V)}$$

and since each part can be integrated independently, we can estimate  $e^{\tau X_T}$  and  $e^{\tau X_V}$  directly. However, in general  $[X_T, X_V] \neq 0$  and therefore

$$e^{\tau(X_T + X_V)} \sim e^{\tau X_T} e^{\tau X_V}$$

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<sup>4</sup>The Legendre condition ask for the convexity of the Hamiltonian function for which its Hessian does not vanish.

conicide only in the first term. This becomes a first order method.

In order to obtain higher order methods, we search for coefficients  $\{a_i\}_1^m$  and  $\{b_i\}_1^m$  such that  $\sum_i a_i = 1$  and  $\sum_i b_i = 1$  to estimate  $e^{\tau X_H}$  by the composition of maps

$$e^{\tau X_T + \tau X_V} \sim e^{a_1 \tau X_T} e^{b_1 \tau X_V} \dots e^{a_m \tau X_T} e^{a_m \tau X_V}. \quad (13)$$

We must impose additional conditions to the coefficients  $a_i$  and  $b_i$  for matching more terms on both sides of the expression (13). For that, we use the Baker-Campbell-Hausdorff (BCH) formula and derive a set of polynomial conditions for  $a_i$  and  $b_i$ . In particular, the derivation of time-parallel methods impose a reversibility condition which requires that the symplectic method be symmetric [28].

Using the BCH formula we can write the symplectic integrator (13) of order  $k$  with its residue as

$$e^{\tau X_T + \tau X_V} = e^{a_1 \tau X_T} e^{b_1 \tau X_V} \dots e^{a_m \tau X_T} e^{a_m \tau X_V} + \mathcal{O}(\tau^{k+1}). \quad (14)$$

which implies

$$e^{a_1 \tau X_T} e^{b_1 \tau X_V} \dots e^{a_m \tau X_T} e^{a_m \tau X_V} = e^{\tau X_H} - \mathcal{O}(\tau^{k+1}). \quad (15)$$

The numerical solution follows a modified or “surrounded” Hamiltonian which we consider as the nonautonomous function

$$\tilde{H}(t, q, p) = H(q, p) + t^{k+1} H_1(t, q, p). \quad (16)$$

This property give us a measure for the error committed by the symplectic methods which corresponds to the error Hamiltonian  $\tau^{k+1} H_1(\tau, q, p)$  for fixed  $\tau$ . The interested readers will find a deeper discussion on the subject in the works of Suzuki [47], Yoshida [51] for this type of Hamiltonians and McLachlan [37], Laskar and Robutel [31] for Hamiltonians of the form  $H(q, p) = T(p) + \epsilon V(q)$  for small  $\epsilon$ . A more general discussion on the construction of symplectic integrators using the BCH formula is found in Hairer *et.al.* [22].

For every symplectic integrator obtained with this process, we have a Hamiltonian function (16) characterized by its error Hamiltonian which depends on  $(\{a_i\}, \{b_i\}, \tau)$ , and then an analytical flow  $\varphi^{\tilde{H}} \in \text{Ham}(M, \omega)$  associated to the numerical solution. For  $f, g \in \mathfrak{F}_0(M)$  such that  $f \neq g$  the Hamiltonian maps

$$\varphi^f = e^{\tau X_f} \quad \text{and} \quad \varphi^g = e^{\tau X_g}, \quad \varphi^f, \varphi^g \in \mathcal{H}(M, \omega), \quad (17)$$

associated to their flows fulfills  $\varphi^f \neq \varphi^g$ . The Hofer’s metric give us a way to measure the distance between them in  $\text{Ham}(M, \omega)$ . This fact permit us to compare symplectic integrators in an geometrical framework.

## 5 Time-parallel integrators

The corner stone in the theory of time-parallel integrators is the use of two different numerical flows, generally using a two level discretization  $\delta t \prec \Delta t \prec$

$[0, T]$  and a corrector step which propagates sequentially with the coarse flow, the values obtained in parallel with the fine flow. In the seminal article of Nievergelt [39] he proposed, as an example, using the Euler method on each discretization. This produces two numerical flows which interplays to estimate the final sequential solution.

The first documented proposal for a time-parallel algorithm for Hamiltonian systems (using a symplectic integrator), is in the work of Saha, Stadel and Tremain [44]. They propose a time-parallel algorithm for almost integrable Hamiltonian systems in action-angle coordinates. In such type of coordinates, the integrable part of the system corresponds to the actions which are constants in the flow. Instead of having a two level discretization, they use a single level discretization with two flows: one for the integrable system and the other one for the complete (perturbed) system using the symplectic mid-point rule. In this work, at least from the examples they show, it is not possible to use a high order symplectic method.

The next interesting proposal is the Parareal algorithm which was used for Hamiltonian systems with a lot of degrees of freedom [2, 10, 14]. However, for long time simulations of systems with a few degrees of freedom Parareal has not a well behavior [14, 15]. The problem is that the parareal algorithm (in fact, the parareal step) does not preserves the symplecticity when it propagates the fine flow with the coarse one. There are several attempts to obtain a better corrector step in order to preserve the symplecticity [5, 12, 28], however, there are not a concrete answer to this problem. Here we ask for an additional point.

Given two different symplectic maps, one for each discretization we can obtain the symplectic map of its Lie bracket and construct a symplectic corrector as in [5, 28]. At each iteration corresponds a point in  $\text{Ham}(M, \omega)$  and then there exists a Hamiltonian isotopy  $h_t \subset \text{Ham}(M, \omega)$  which contains all such points. Since the fine flow is given (it corresponds to the final numerical solution we expect to approximate), the question rests in the choice of the coarse flow in order to approach the fine solution in the minimal number of iterations. We give a partial answer in the next paragraphs.

Let's consider the initial value problem

$$\dot{y}(t) = X_H(y(t)), \quad y(0) = y_0. \quad (18)$$

where  $y : [0, T] \rightarrow M$  and  $X_H \in \mathfrak{ham}(M, \omega)$ . We discretize the problem by partitioning  $[0, T]$  in  $N$  subintervals of size  $\Delta t = T/N$  which we call *branches* as in [39]. We set  $t_0 = 0$ ,  $t_n = T$  and  $t_i = i\Delta t$  such that

$$0 = t_0 < t_1 < t_2 < \dots < t_i < \dots < t_N = T. \quad (19)$$

We write  $\Delta t \prec [0, T]$  for this partition. Each branch in  $\Delta t$  is decomposed in  $N_\delta \in \mathbb{N}$  subintervals  $\delta t = \Delta t/N_\delta$  which corresponds to the final resolution. Then  $\delta t \prec \Delta t \prec [0, T]$ .

On this discretization we introduce two levels of resolution: a coarse symplectic solver  $G$  on the  $\Delta t$  resolution and a fine symplectic solver  $F$  on the  $\delta t$

one. Their flows  $\varphi^G$  and  $\varphi^F$  are defined uniquely by their coefficients and their timesteps  $(\{a_i\}, \{b_i\}, \Delta t)$  and  $(\{c_i\}, \{d_i\}, \delta t)$  respectively.

The fine and the coarse propagation of the solutions  $y_n$  on a branch are respectively given by  $\mathcal{F}(y_n)$  and  $\mathcal{G}(y_n)$ . For the problem (18) we estimate the first guess sequence with the coarse solver  $y_0^{(0)} = y(0)$  and  $y_{n+1}^{(0)} = \mathcal{G}(y_n^{(0)})$ . The time-parallel algorithms are given by some variation of the two steps

$$y_0^{(k+1)} = y_0^{(k)}, \quad (20)$$

$$y_{n+1}^{(k+1)} = \Gamma \left( \mathcal{F} \left( y_n^{(k)} \right), \mathcal{G} \left( y_n^{(k+1)} \right), \mathcal{G} \left( y_n^{(k)} \right) \right), \quad (21)$$

where the subscripts are the propagation in time and the superscripts are the iterations. In (21),  $\Gamma$  is the corrector which is an operator on the symplectic solvers. The general algorithm is as follows

**Time-parallel algorithm 1.**

- 1: Setup of the initial guess sequence
- 2:  $y_0^0 = y(0)$ ,  $y_{n+1}^0 = \mathcal{G}(y_n^0)$
- 3: For  $k = 1$  to  $k_{max}$
- 4:     Parallel resolution on  $[T^n, T^{n+1}]$ :
- 5:         compute  $\mathcal{F} \left( y_n^{(k)} \right)$ ,
- 6:         For  $n = k$  to N
- 7:             Sequential corrections:
- 8:                 compute  $y_{n+1}^{(k+1)} = \Gamma \left( \mathcal{F} \left( y_n^{(k)} \right), \mathcal{G} \left( y_n^{(k+1)} \right), \mathcal{G} \left( y_n^{(k)} \right) \right)$ .
- 9:         end for (n).
- 10:        end for (k).

In particular the parareal algorithm implements (21) as

$$y_{n+1}^{(k+1)} = \mathcal{F} \left( y_n^{(k)} \right) + \mathcal{G} \left( y_n^{(k+1)} \right) - \mathcal{G} \left( y_n^{(k)} \right). \quad (22)$$

Expression (22) has been called *the parareal iteration*.

Recall that the construction of a symplectic corrector uses the Lie bracket of  $X_F$  and  $X_G$  with at least one reversal integration, then we impose that both symplectic solvers be symmetrical [28].

Every implicit symplectic integrator for separable Hamiltonian systems can be uniquely determined by its coefficients  $\{c_i\}$  and  $\{d_i\}$ . Its numerical flow  $\varphi^{\tilde{H}}$  by the coefficients and the timestep  $(\{c_i\}, \{d_i\}, \tau)$ . Then, we identify the flow of every symplectic integrator with timestep  $\tau$  with the triplet  $\varphi^{\tilde{H}} \cong (\{c_i\}, \{d_i\}, \tau)$ . Suppose that we have, as the fine symplectic scheme of order  $k$ , the more accumulated integrator in the family of the  $k$ -order symplectic integrators.

**Theorem 1.** *Given the two level discretization  $\delta t \prec \Delta t \prec [0, T]$  and the final (optimal) symplectic integrator  $(\{c_i\}, \{d_i\}, \delta t)$  with flow  $\varphi^F$  the closest flow  $\varphi^G$  in  $\text{Ham}(M, \omega)$  for  $\Delta t$  is given by  $(\{c_i\}, \{d_i\}, \Delta t)$ .*

*Proof.* Immediate using the triangle's inequality property of the Hofer's metric.  $\square$

As a consequence, the use of some symplified symplectic scheme increases the number of iterations and, in general, introduces an erratic behavior since the dynamics of both flows is in general not equivalent.

In this case, the corrector step constructed by the author in [28] coincides with those studied by Wisdom and Holman [50] McLachlan [36] and Laskar and Robutel [31].

There are more results from the symplectic topology which apply for particular families of Hamiltonians. For example, a function  $H \in \mathfrak{F}_0(M, \omega)$  is called to have *quadratic growth* if there exists  $c \in \mathbb{R}$  finite such that  $|d^2H(z)| < c$  for all  $z \in M$ . For such functions, the Hamiltonian isotopy of the Theorem 1 is a geodesic in  $\text{Ham}(M, \omega)$  [35, Ch. 12].

## 6 A numerical test

We compare the pure parareal with the more accurate JL11 algorithm introduced in [26] for the one dimensional Spin-orbit problem with several values of the parameter  $\alpha$

$$H(q, p) = \frac{1}{2}p^2 - \varepsilon(\cos(2q) + \alpha(\cos 2q + \theta - 7\cos 2q - \theta)) \quad (23)$$

We select a 8th order symplectic integrator from the  $\mathcal{S}\mathcal{B}\mathcal{A}\mathcal{B}_n$  family for both  $\mathcal{F}$  and  $\mathcal{G}$  solvers.

The first approximation with the coarse solver approach faster than the symplectic proposed in [28] and JL11 proposed in [26]. However, as was showed in the later document, JL11 obtain exactly the same sequential solution.

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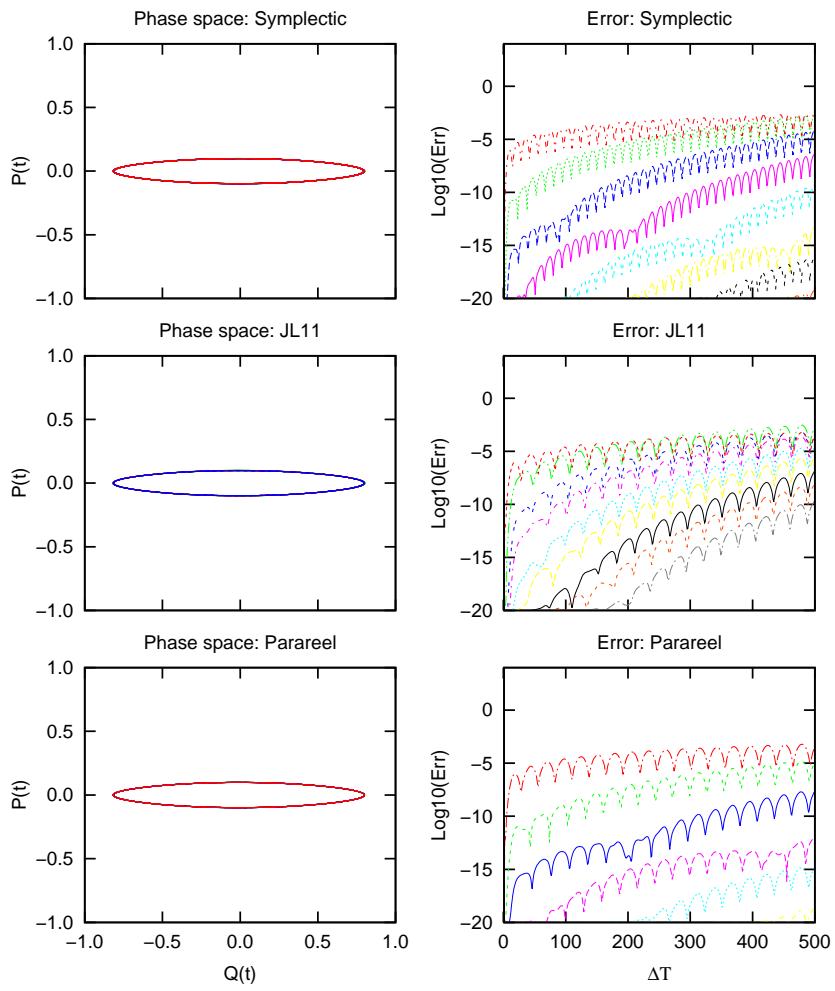


Figure 1: Numerical test of the Spin-orbit problem with JL11 and parareal. The parameters are  $\varepsilon = 0.1$ ,  $\alpha = 0.01$ ,  $\theta = 0.2$ ,  $\delta t = 1/128$ ,  $\Delta t = 1$ ,  $p_0 = 0$ ,  $q_0 = 0.8$ .